

# Local electronic structure and inhomogeneity in heavy fermion systems

Jian-Xin Zhu  
Los Alamos National Laboratory

QDM 2015, Santa Fe, Mar. 9, 2015



## Collaborators:

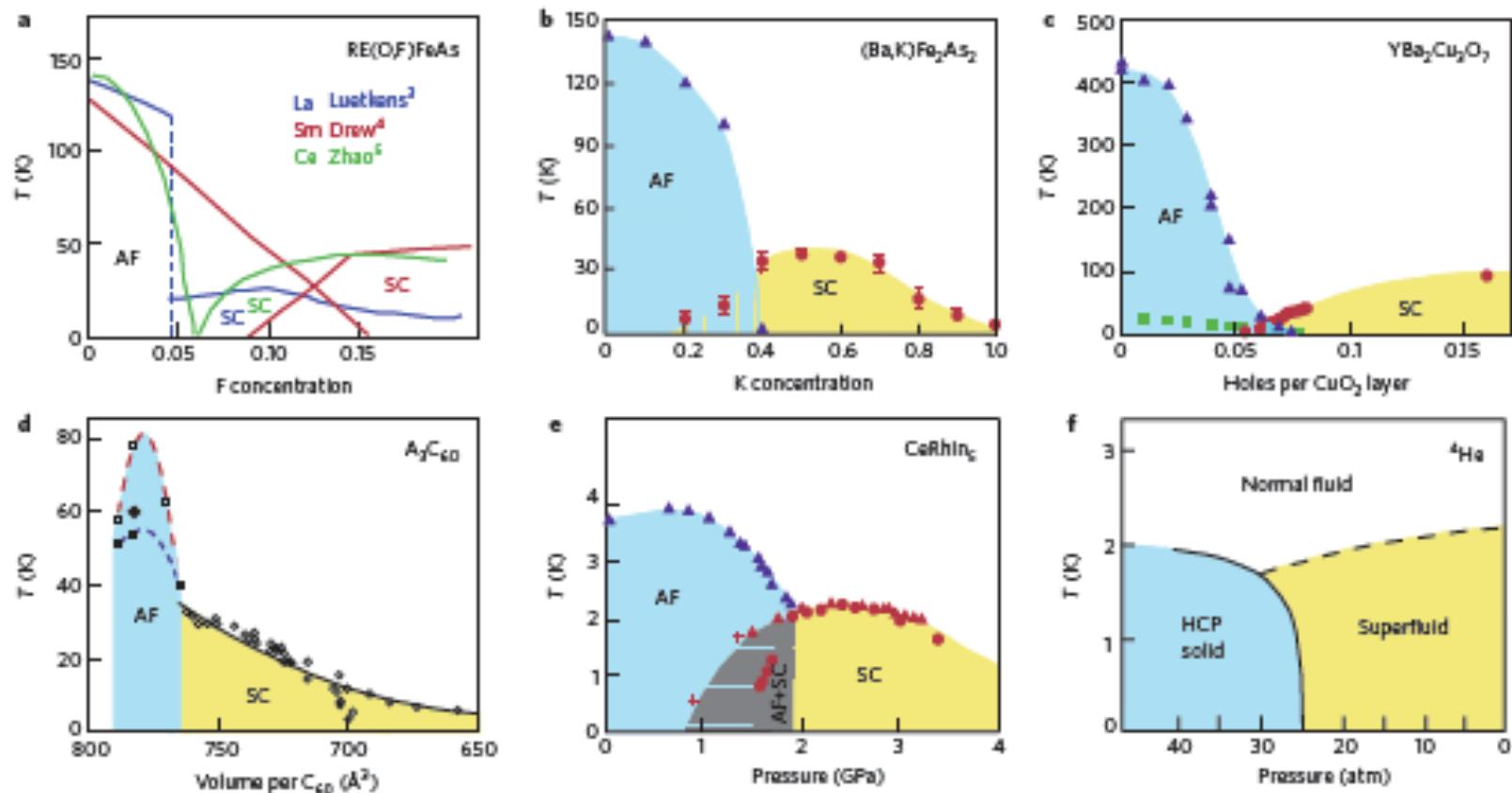
Jean-Pierre Julien (UJF)  
Joseph Wang (LANL)  
Ivar Martin (ANL)  
Alan R. Bishop (LANL)  
Yoni Dubi (Ben Gurion)  
Sasha Balatsky (LANL)

Supported by DOE BES Program  
LANL-LDRD

# Outline

- Emergent phenomena and electronic inhomogeneity in correlated electron systems
- Staggered Kondo Phase
- Local electronic structure in Kondo hole
- Local electronic structure around a single impurity in topological Kondo insulators
- Summary

# Quantum materials exhibits novel electronic phases



- These phases characterize the states of electrons.
- Superconductivity is in close proximity to AF magnetism.
- Ground state in different phases can be tuned by control parameters.

# They emerge from competing interactions!

- Several brands

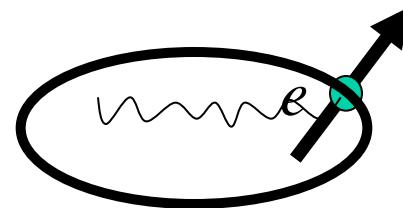
Charge?

Spin?

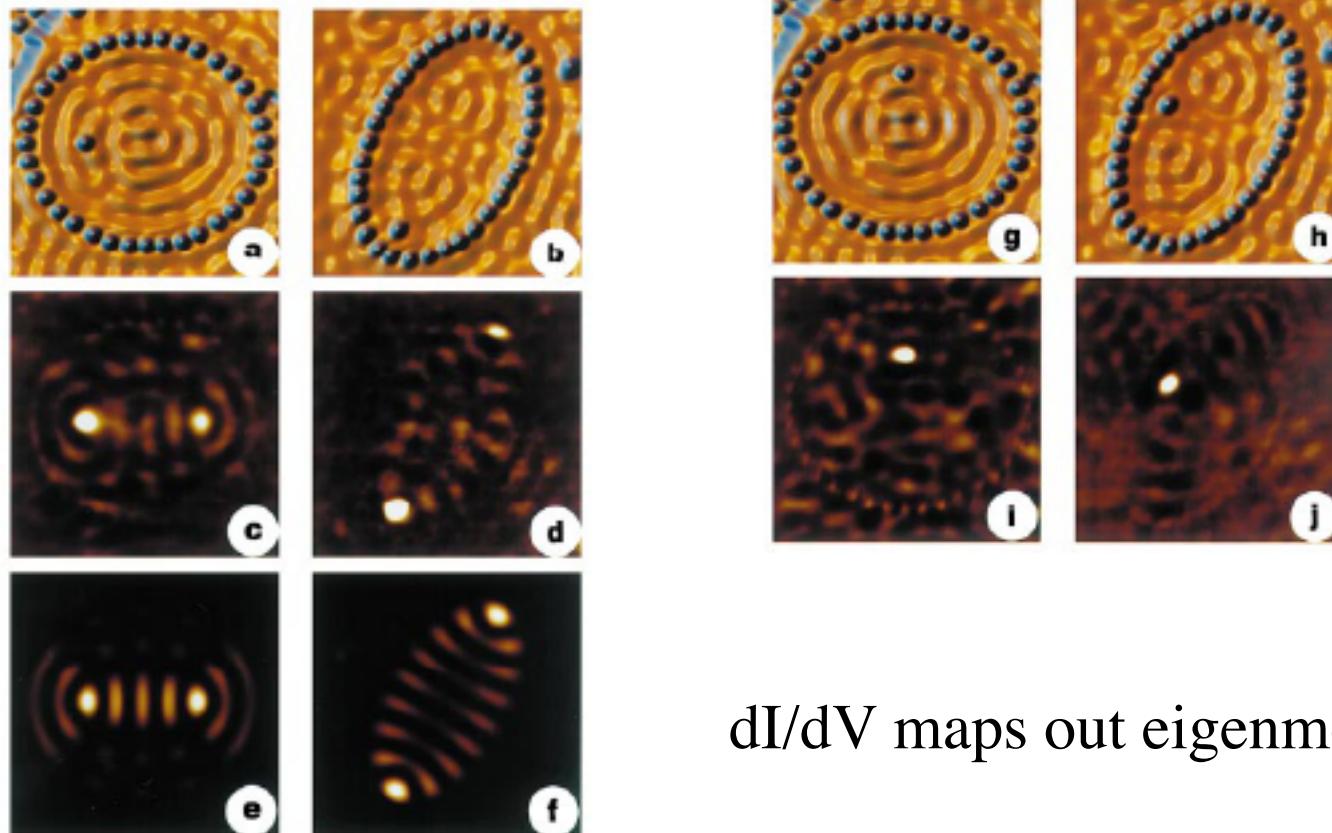
Lattice?

Orbital?

- Several competing interactions (kinetic energy, Coulomb energy, electron-lattice coupling)
- Rich selection of competing orders and transitions between them. Consequently, immense tunability, especially near the transition.
- Electronic inhomogeneity important consequence of competition.

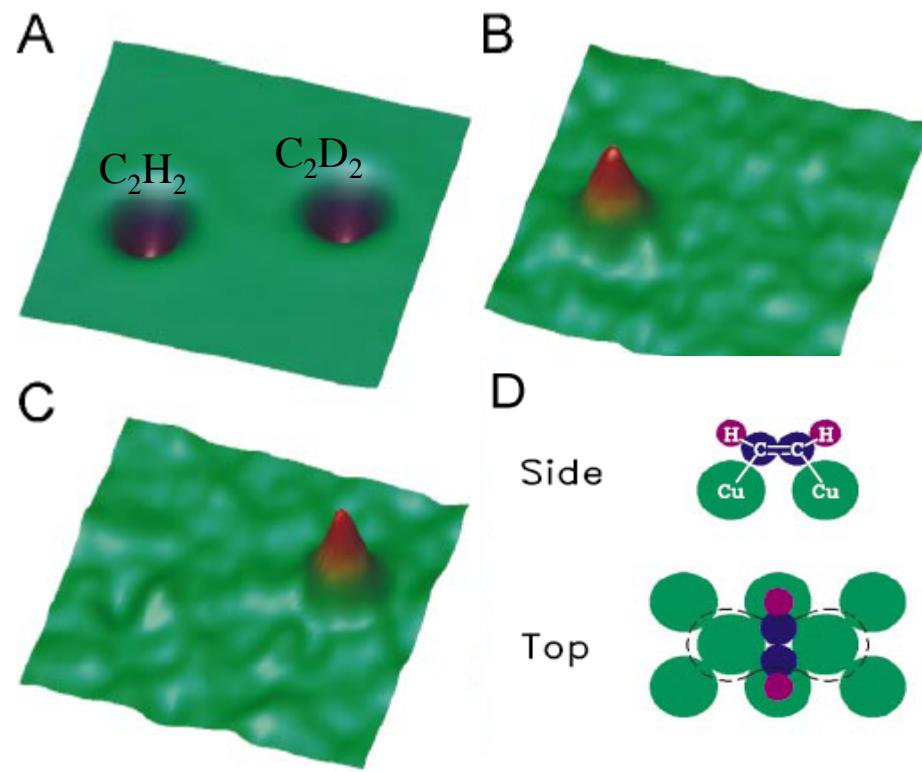


# Quantum mirages formed by coherent project of electronic structure



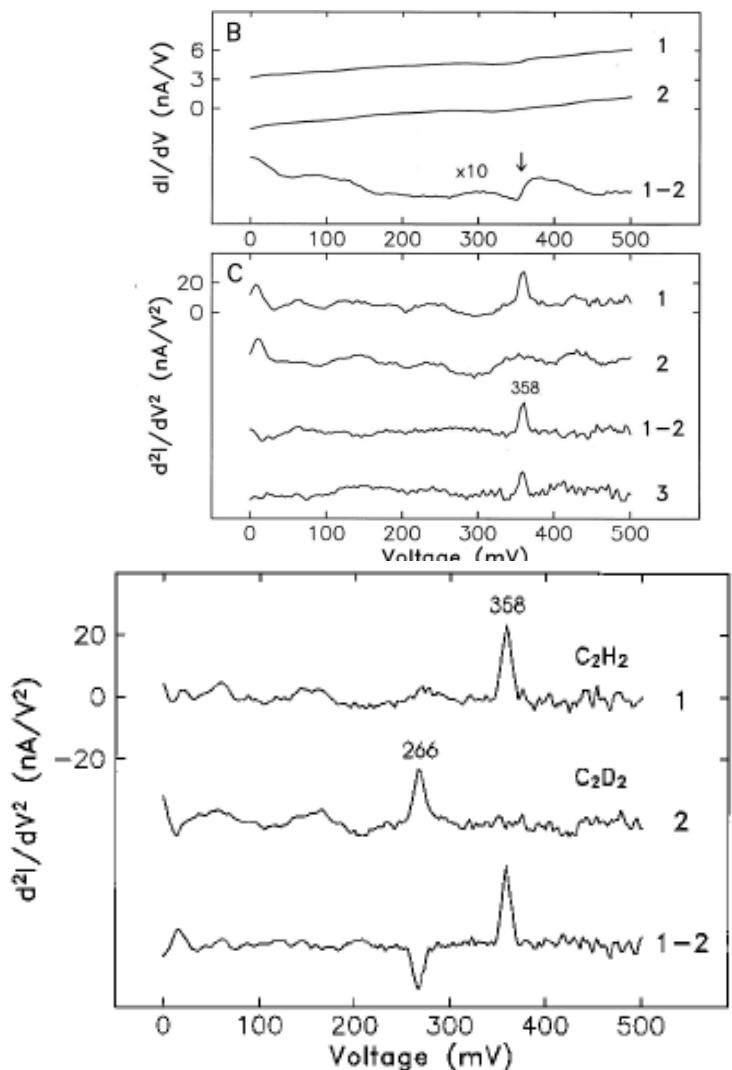
H. C. Manoharan *et al.*, Nature **403**, 512 (2000)

# IETS-STM observation of local inelastic scattering model



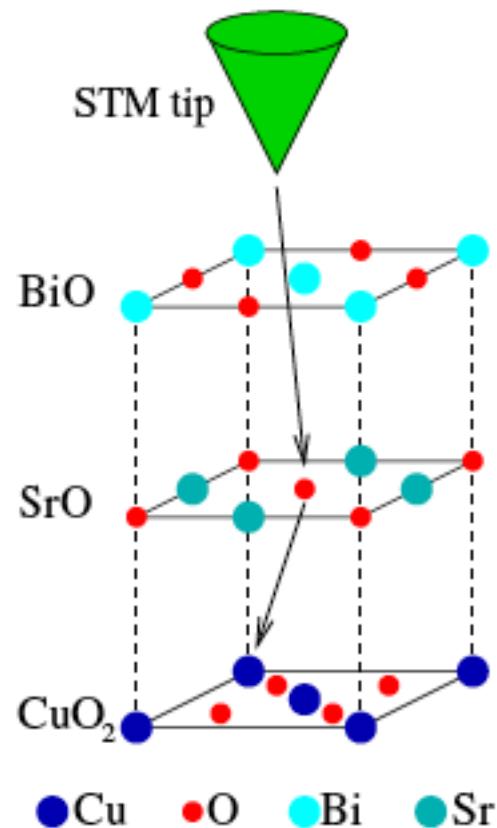
$C_2H_2$ : acetylene

$C_2D_2$ : deuterated acetylene

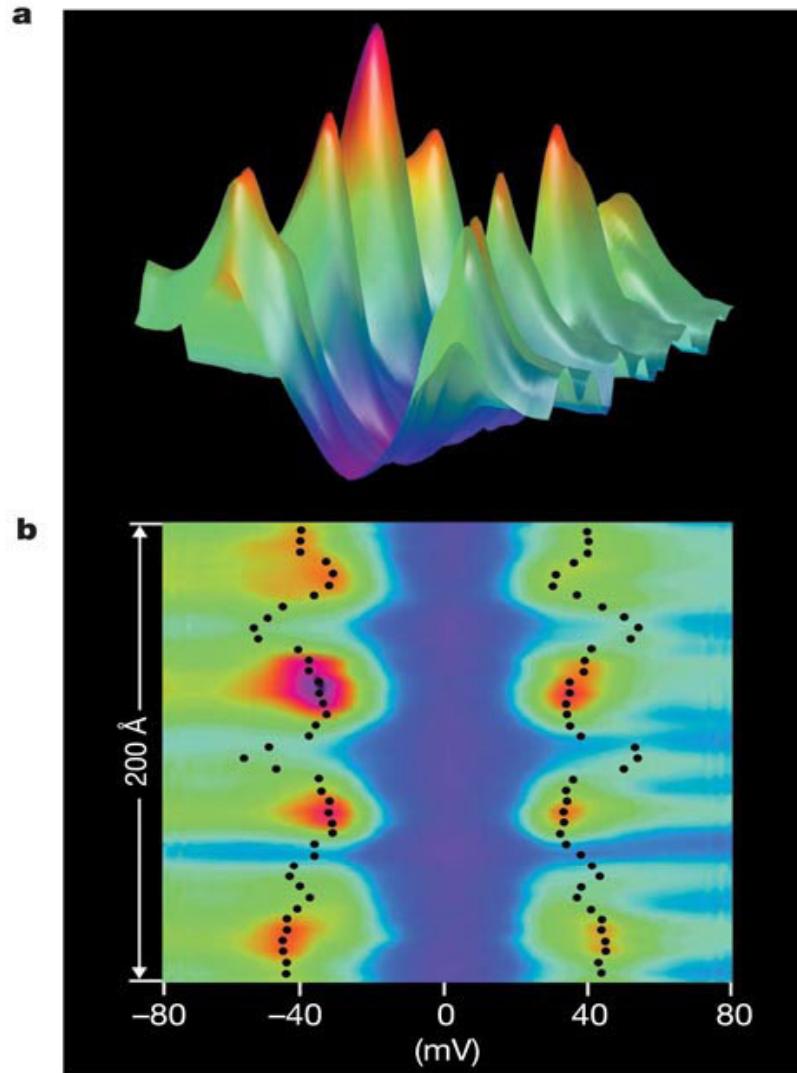


Stipe, Rezaei & Ho, Science 280, 1732 (1998)  $d^2I/dV^2$  maps out the vibration mode!

# Experimental evidence for electronic inhomogeneity in cuprates

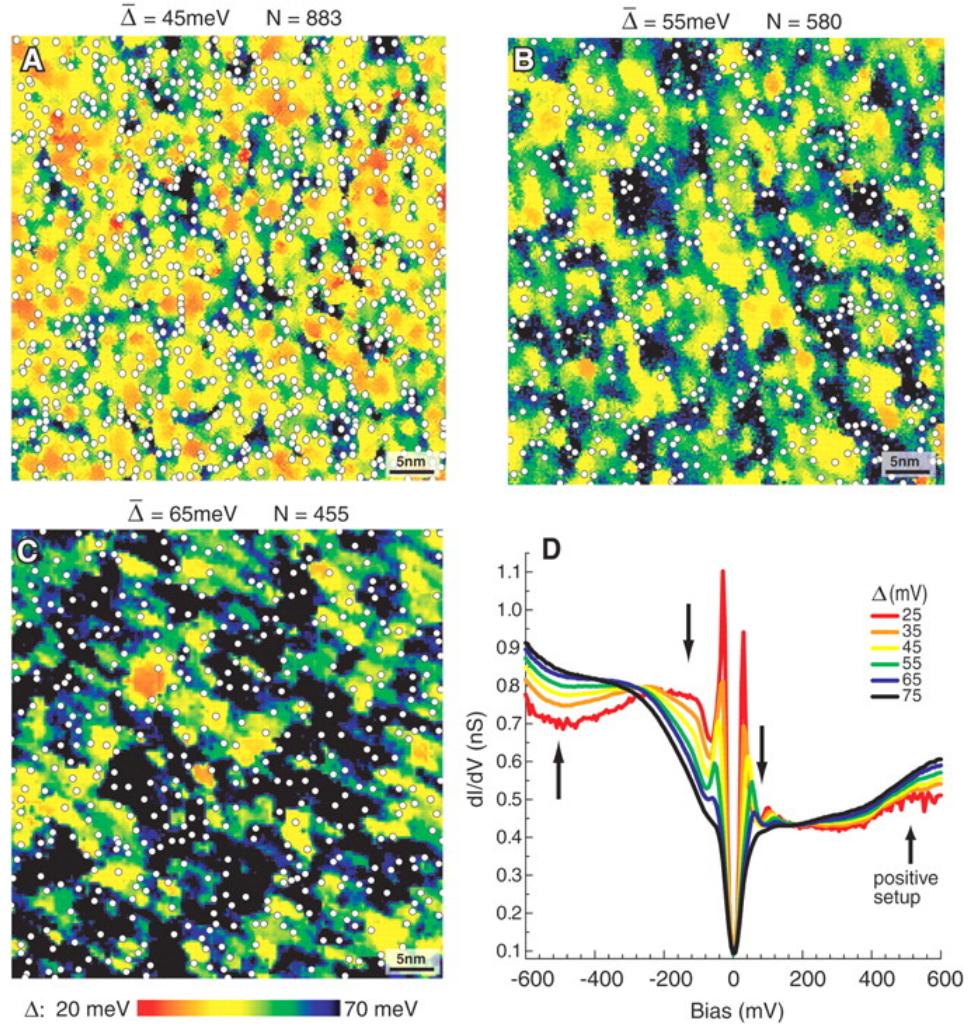


1. Spectra gap varies dramatically on the length scale of 50 Angstrom.
2. “Coherence peak” positions are symmetric about zero bias.
3. Coherent peak intensity is suppressed in the wide gap regions.
4. Low energy part of the tunneling spectra are extremely homogeneous.



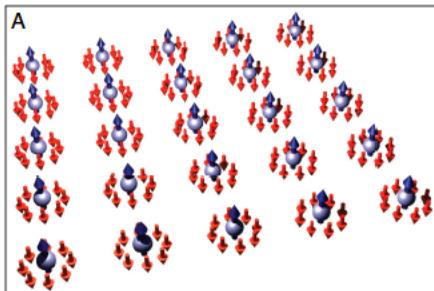
S. H. Pan et al., Nature **413**, 282 (2001)

1. Large gap regions are positively correlated with the oxygen dopants.
2. A charge density variations are significantly weak.
3. Oxygen dopants are interstitial

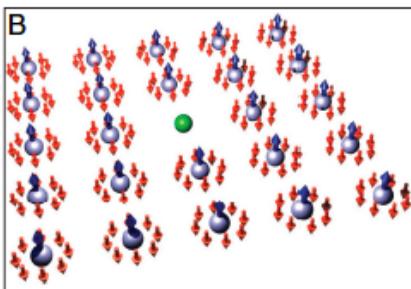


McElroy *et al.*, Science **309**, 1048  
(‘05)

# Applications of STM to heavy fermion systems



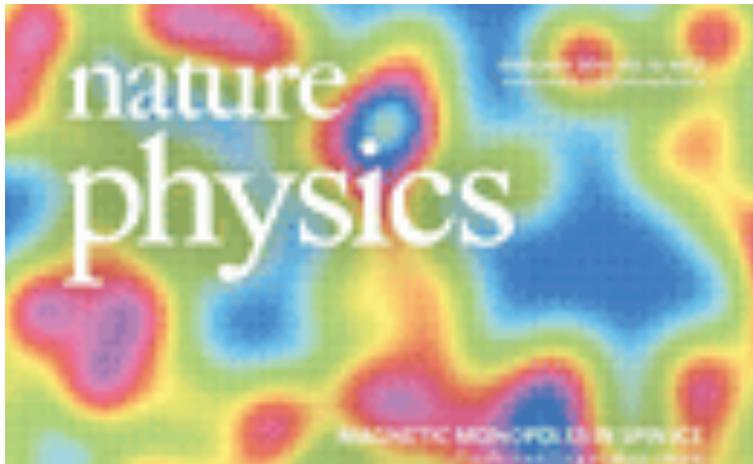
Perfect correlated electron lattice



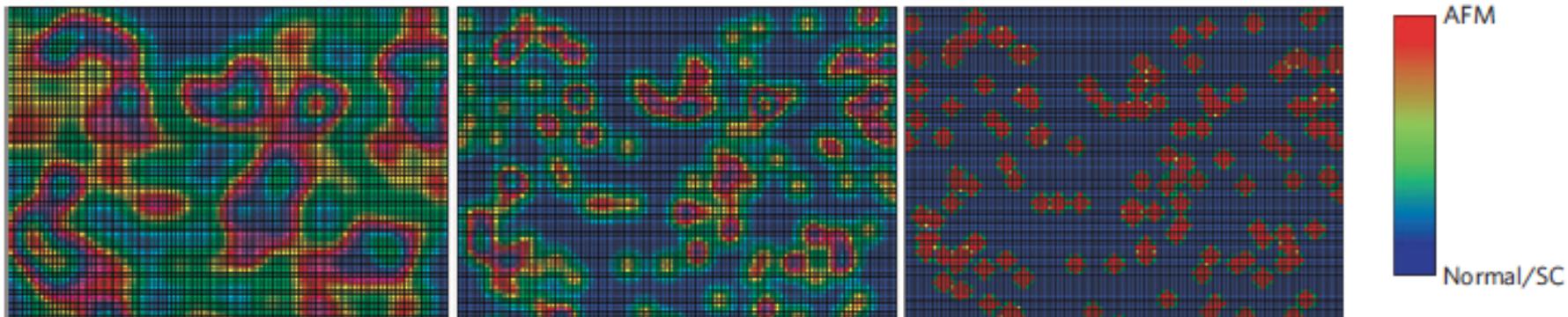
Kondo hole system

- Fano interferene, Kondo lattice formation, and ‘hidden order’ transition in  $\text{URu}_2\text{Si}_2$ 
  - Schmidt et al., Nature **465**, 570 (2010)
  - Aynajian et al., PNAS **107**, 10383 (2010)
- Emerging local Kondo screening and spatial coherence in the heavy-fermion metal  $\text{YbRh}_2\text{Si}_2$ 
  - Ernst et al., Nature **474**, 362 (2011)
- Kondo holes in  $\text{U}_{1-x}\text{Th}_x\text{Ru}_2\text{Si}_2$ 
  - Hamidian et al., PNAS **108**, 18233 (2011)

# Evidence of inhomogeneity in CeRh(In<sub>1-x</sub>Cd<sub>x</sub>)<sub>5</sub>



- Puddle size shrinks with increased pressure.  
Seo *et al.*, Nat. Phys. **10**, 120 (2014)

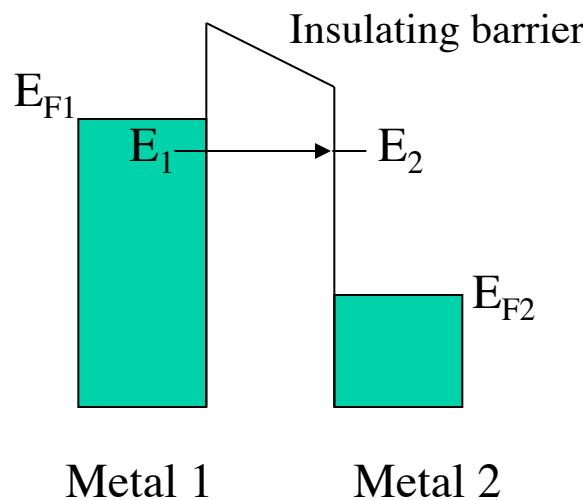


Pressure

# Connection between theory and experiment

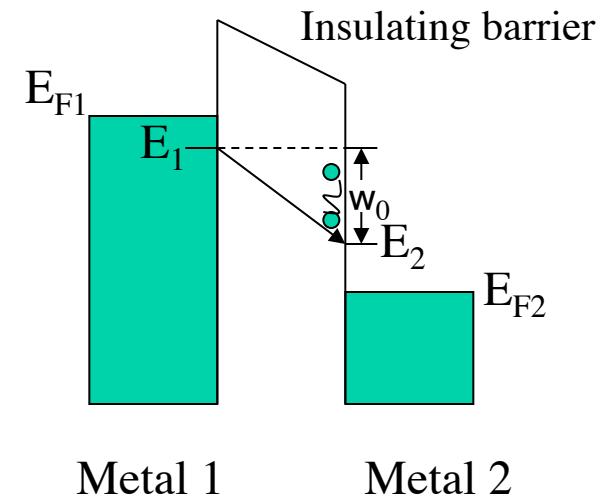
|                                 |                                    |                       |                                   |                            |
|---------------------------------|------------------------------------|-----------------------|-----------------------------------|----------------------------|
| STM<br>tunneling<br>conductance | $\frac{dI}{dV}(\mathbf{r}, V)$     | $\longleftrightarrow$ | $\rho(\mathbf{r}, E)$             | Local density<br>of states |
|                                 | $\frac{d^2I}{dV^2}(\mathbf{r}, V)$ |                       | $\frac{d\rho}{dE}(\mathbf{r}, E)$ |                            |

Elastic tunneling



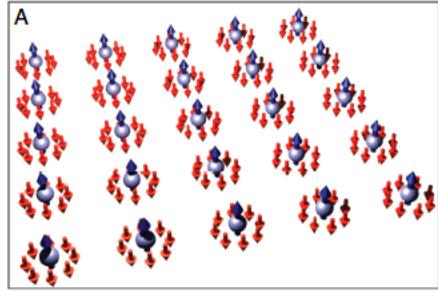
$$E_1 = E_2$$

Inelastic tunneling



$$E_1 = E_2 + w_0$$

# Kondo stripe in Anderson-Heisenberg model



Perfect correlated electron lattice

$$\begin{aligned}
 H = & -\sum_{ij,\sigma} \left( t_{ij}^c + \mu \delta_{ij} \right) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} \left[ V_{cf} c_{i\sigma}^\dagger f_{i\sigma} + \text{H.c.} \right] \\
 & + \sum_{i,\sigma} \left( \epsilon_f - \mu \right) f_{i\sigma}^\dagger f_{i\sigma} + \sum_i U_f n_{i\uparrow}^f n_{i\downarrow}^f + \frac{J_H}{2} \sum_{ij} \left( S_i \cdot S_j - \frac{n_i^f n_j^f}{4} \right)
 \end{aligned}$$

Slave-boson approach for  $U_f \rightarrow \infty$      $f_{i\sigma} = \tilde{f}_{i\sigma} b_i^\dagger$

$$\tilde{f}_{i\sigma}^\dagger \tilde{f}_{i\sigma} + b_i^\dagger b_i = 1$$

MFA:  $b_i$  treated as a c-number

$$H_{eff} = -\sum_{ij,\sigma} \left( t_{ij}^c + \mu \delta_{ij} \right) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} \left[ V_{cf} b_i c_{i\sigma}^\dagger \tilde{f}_{i\sigma} + \text{H.c.} \right] - \sum_{ij,\sigma} \left( \chi_{ij} - (\epsilon_f + \lambda_{i\sigma} - \mu) \delta_{ij} \right) \tilde{f}_{i\sigma}^\dagger \tilde{f}_{i\sigma}$$

# Anderson-Bogoliubov-de Gennes Equations

$$\sum_j \begin{pmatrix} h_{ij}^c & \Delta_{ij} \\ \Delta_{ji}^* & h_{ij}^f \end{pmatrix} \begin{pmatrix} u_{j\sigma}^n \\ v_{j\sigma}^n \end{pmatrix} = E_n \begin{pmatrix} u_{i\sigma}^n \\ v_{i\sigma}^n \end{pmatrix}$$

$$h_{ij}^c = -t_{ij}^c - \mu \delta_{ij},$$

$$\Delta_{ij} = V_{cf} b_i \delta_{ij}$$

$$h_{ij}^f = -\chi_{ij} + [\varepsilon_f + \lambda_{i\sigma} - \mu] \delta_{ij}$$

Numerical details:

Supercell technique [JXZ et al., PRB **59**, 3353 (1999)]

T=0.01,  $\chi=0.1$  (input parameter)

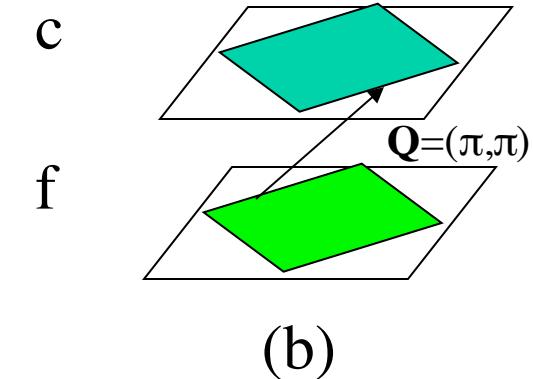
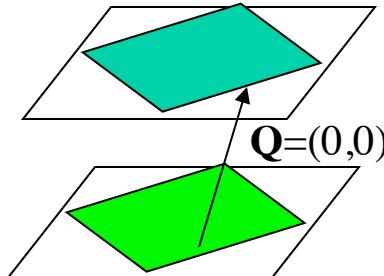
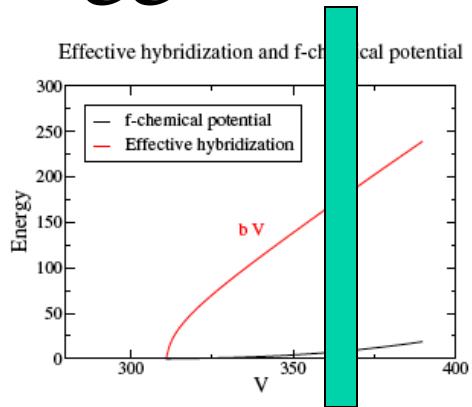
N×N=24×24



JXZ, Martin, Bishop, PRL **100**, 236403 (2008)



# Staggered Kondo Phase in the PM regime



(a) Normal Kondo Phase

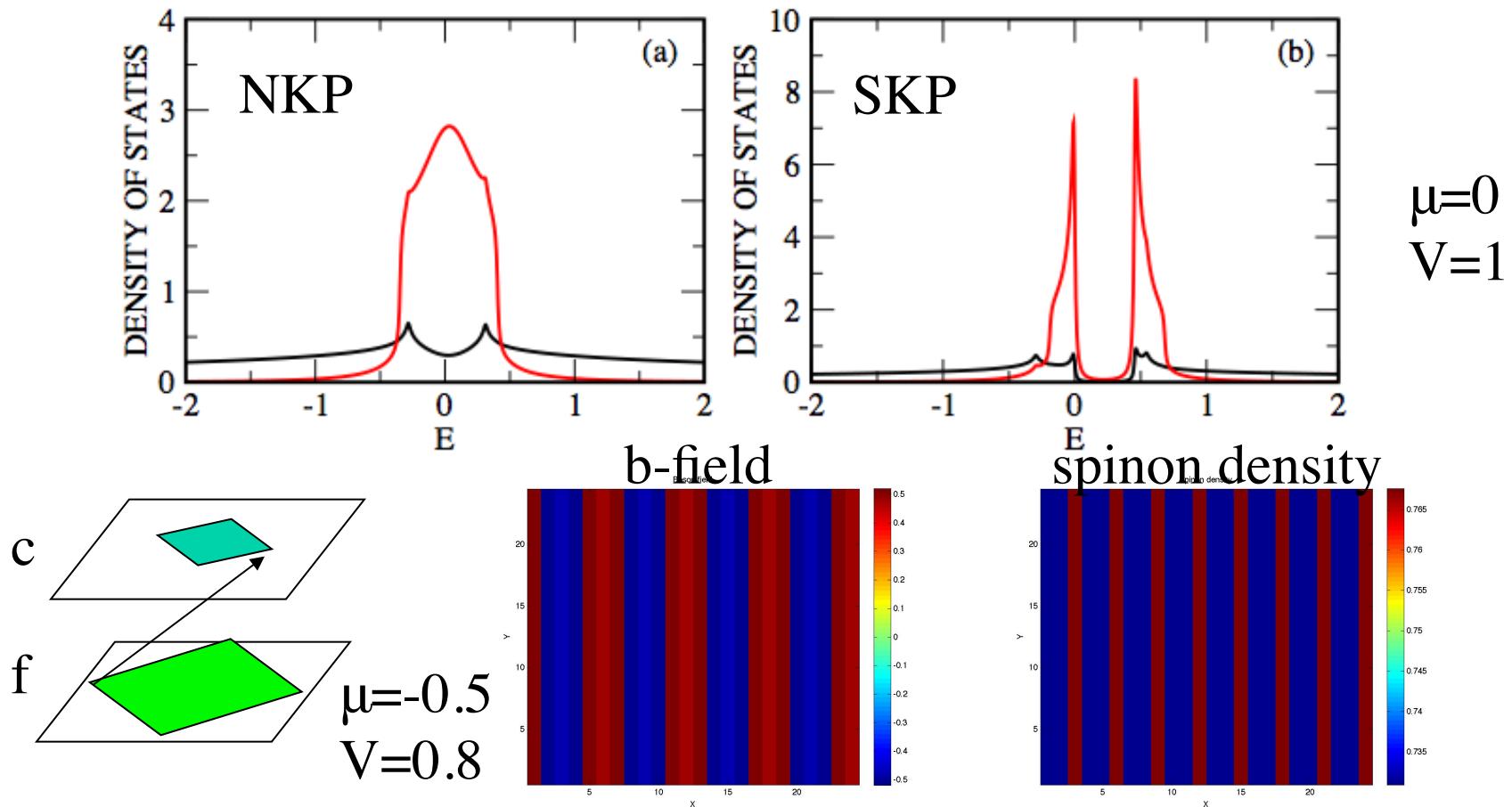
$$b_i = b_0$$

(b) Staggered Kondo Phase

$$b_i = b_0(-1)^{(ix+iy)}$$

In an infinite-U Anderson-Heisenberg model,  
SKP is lower in energy than NKP for a  
uniform RVB OP  $\chi > 0$  and vice versa.

# Spinon spectral density for NKP and SKP phases for $\chi>0$

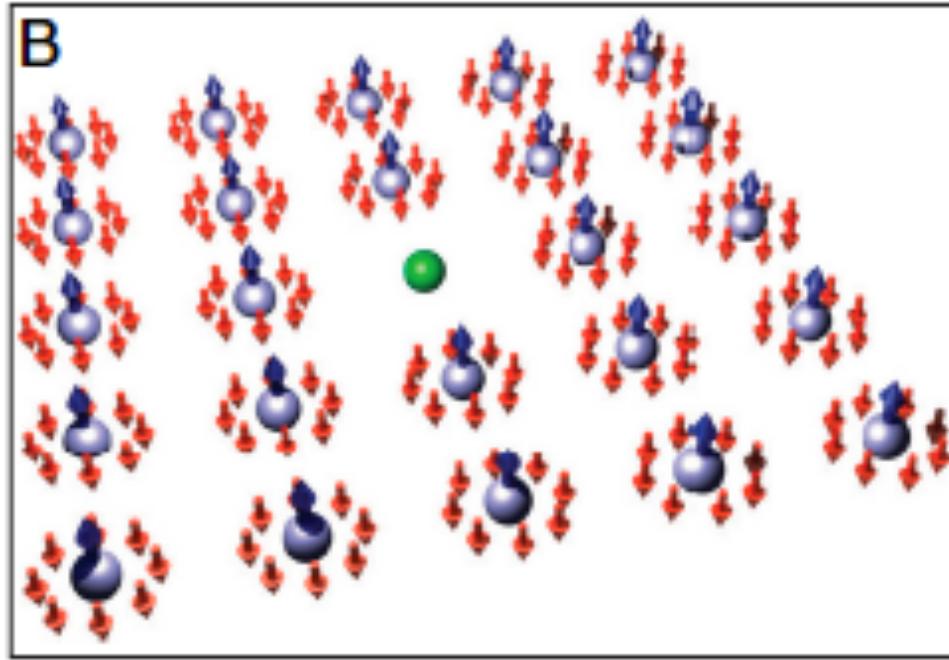


In the presence of strong mismatch between c- and f-patch of fermi topology, even a Kondo stripe phase is possible!

JXZ, Martin, Bishop, PRL **100**, 236403 (2008)



# Kondo Hole Model



$$H = H_0 + H_{imp}$$

$$H_0 = - \sum_{ij,\sigma} (t_{ij}^c + \mu \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} [V_{cf} c_{i\sigma}^\dagger f_{i\sigma} + \text{H.c.}] + \sum_{i,\sigma} (\varepsilon_f - \mu) f_{i\sigma}^\dagger f_{i\sigma} + \sum_i U_f n_{i\uparrow}^f n_{i\downarrow}^f$$

$$H_{imp} = \sum_\sigma \varepsilon_c^I c_{I\sigma}^\dagger c_{I\sigma} + \sum_\sigma (\varepsilon_f^I - \varepsilon_f) f_{I\sigma}^\dagger f_{I\sigma} + \sum_\sigma [(V_{cf}^I - V_{cf}) c_{I\sigma}^\dagger f_{I\sigma} + \text{H.c.}] - U_f n_{I\uparrow}^f n_{I\downarrow}^f$$

Kondo hole: Level at  $\varepsilon_f^I$  unoccupied

# Density-matrix Gutzwiller approx.

$$H_{eff} = H_0 + H_{imp}$$

$$\widetilde{H}_0 = - \sum_{ij,\sigma} (t_{ij}^c + \mu \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} [V_{cf} g_{i\sigma} c_{i\sigma}^\dagger \tilde{f}_{i\sigma} + \text{H.c.}] + \sum_{i,\sigma} (\varepsilon_f + \lambda_{i\sigma} - \mu) \tilde{f}_{i\sigma}^\dagger \tilde{f}_{i\sigma} + \sum_i U_f d_i + Cont$$

$$H_{imp} = \sum_{\sigma} \varepsilon_c^I c_{I\sigma}^\dagger c_{I\sigma} + \sum_{\sigma} (\varepsilon_f^I - \varepsilon_f) \tilde{f}_{I\sigma}^\dagger \tilde{f}_{I\sigma} + \sum_{\sigma} [(V_{cf}^I - V_{cf}) c_{I\sigma}^\dagger \tilde{f}_{I\sigma} + H.c.] - U_f$$

$g_{i\sigma}$  ( $\sim \sqrt{q_i}$  <sup>a</sup>): Local renormalization parameter

$$g_{i\sigma} = \left[ \frac{\left( \bar{n}_{i\sigma}^{\tilde{f}} - d_i \right) \left( 1 - \bar{n}_i^{\tilde{f}} + d_i \right)}{\bar{n}_{i\sigma}^{\tilde{f}} \left( 1 - \bar{n}_{i\sigma}^{\tilde{f}} \right)} \right]^{1/2} + \left[ \frac{d_i \left( \bar{n}_{i\sigma}^{\tilde{f}} - d_i \right)}{\bar{n}_{i\sigma}^{\tilde{f}} \left( 1 - \bar{n}_{i\sigma}^{\tilde{f}} \right)} \right]^{1/2}$$

$$U \rightarrow \infty : g_{i\sigma} = \left[ \frac{1 - \bar{n}_i^{\tilde{f}}}{1 - \bar{n}_{i\sigma}^{\tilde{f}}} \right]^{1/2}$$

$\lambda_{i\sigma}$ : Lagrange multiplier  
 $d_i$ : double occupation

} subject to constraint

$$\lambda_{i\sigma} = V_{cf} \sum_{\sigma'} \frac{\partial g_{i\sigma'}}{\partial \bar{n}_{i\sigma}^{\tilde{f}}} \left( \langle c_{i\sigma'}^\dagger \tilde{f}_{i\sigma'} \rangle + \text{c.c.} \right)$$

$$-U_f = V_{cf} \sum_{\sigma'} \frac{\partial g_{i\sigma'}}{\partial d_i} \left( \langle c_{i\sigma'}^\dagger \tilde{f}_{i\sigma'} \rangle + \text{c.c.} \right)$$



<sup>a</sup>J.-P. Julien and J. Bouchet, Prog. Theor. Chem. Phys. **15**, 509 (2006)



# Again Anderson-Bogoliubov-de Gennes Equations

$$\sum_j \begin{pmatrix} h_{ij}^c & \Delta_{ij} \\ \Delta_{ji}^* & h_{ij}^{\tilde{f}} \end{pmatrix} \begin{pmatrix} u_{j\sigma}^n \\ v_{j\sigma}^n \end{pmatrix} = E_n \begin{pmatrix} u_{i\sigma}^n \\ v_{i\sigma}^n \end{pmatrix}$$

$$h_{ij}^c = -t_{ij}^c - \mu \delta_{ij} + \varepsilon_I^c \delta_{iI} \delta_{ij},$$

$$\Delta_{ij} = V_{cf} \left[ g_{i\sigma} (1 - \delta_{iI}) + \delta_{iI} \right] \delta_{ij}$$

$$h_{ij}^{\tilde{f}} = \left[ (\varepsilon_f + \lambda_{i\sigma}) (1 - \delta_{iI}) + \varepsilon_I^{\tilde{f}} \delta_{iI} - \mu \right] \delta_{ij}$$

LDOS (Gutzwiller QP):

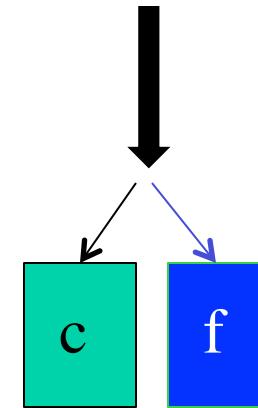
$$(\rho_{i\sigma}^c(E), \rho_{i\sigma}^{c\tilde{f}}(E), \rho_{i\sigma}^{\tilde{f}}(E)) = - \sum_n \left( |u_{i\sigma}^n|^2, u_{i\sigma}^n v_{i\sigma}^n, |v_{i\sigma}^n|^2 \right) \frac{\partial f_{FD}(E - E_n)}{\partial E}$$



# Fano interference

Tunneling conductance measured by STM

- When f-electrons become itinerant, additional transport channel is open



$$\frac{dI}{dV} \Big|_{eV=E} = \frac{2e^2\pi N_0 V_{tc}^2}{\hbar} \sum_{\sigma} \left[ \rho_{i\sigma}^c(E) + 2rg_{i\sigma}\rho_{i\sigma}^{cf}(E) + r^2g_{i\sigma}^2\rho_{i\sigma}^f(E) \right]$$

$$r = V_{tf} / V_{tc}$$

- $g_i$  participates in the Fano interference. Should be any auxiliary field theory

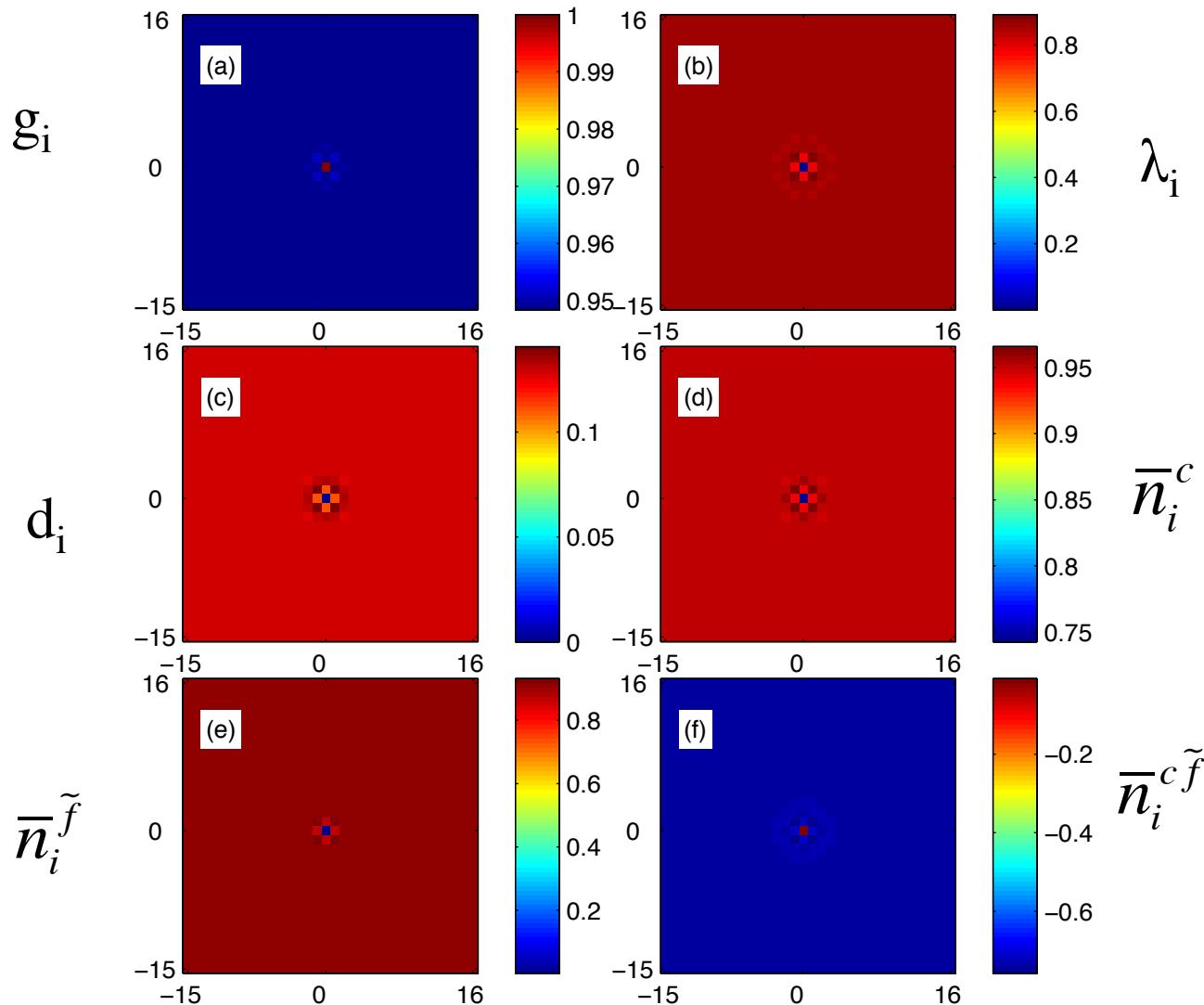
Technical details:

Supercell technique [JXZ et al., PRB **59**, 3353 (1999)]

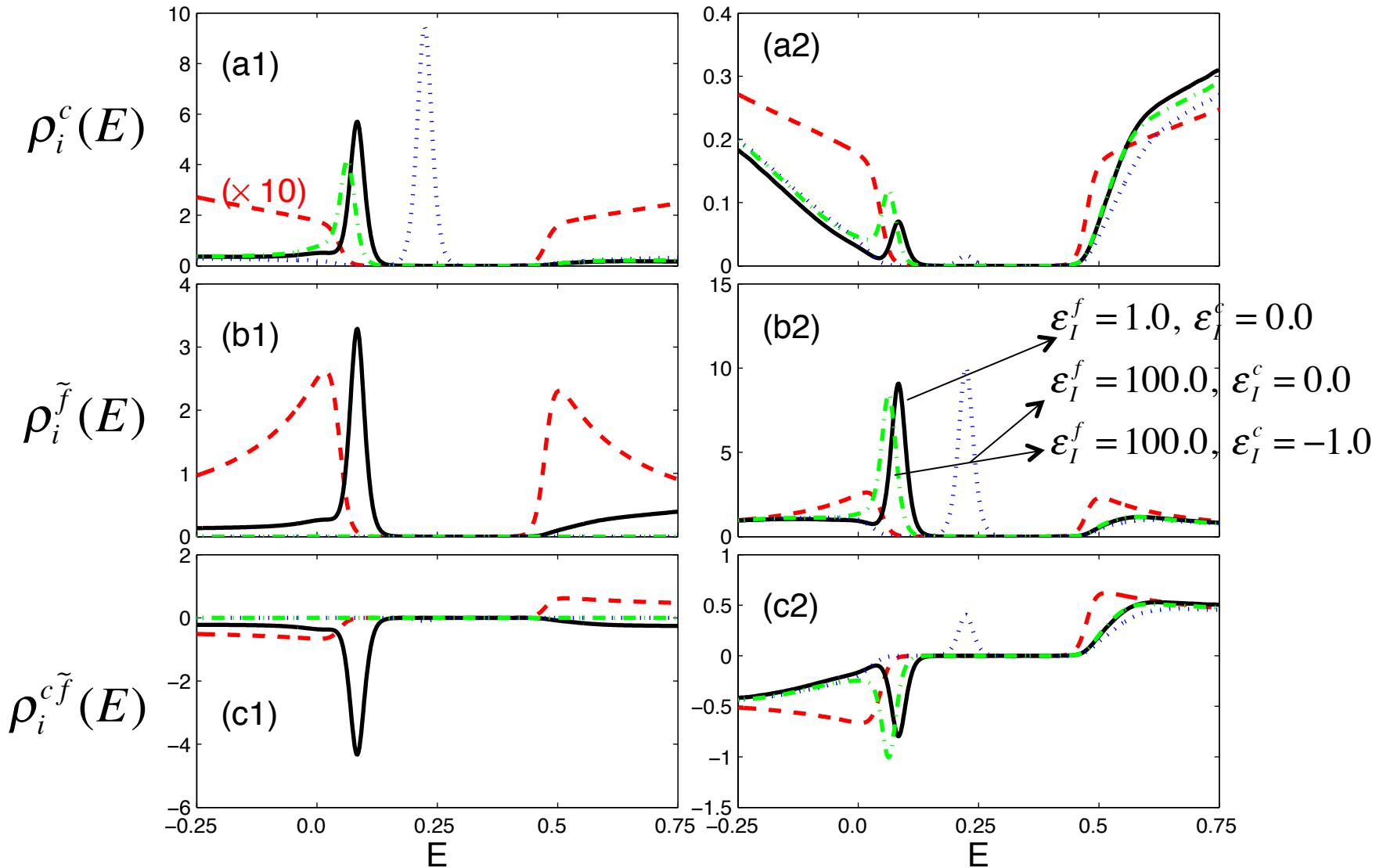
$U=2$ ,  $t^c=1$ ,  $V_{cf}=1.0$ ,  $\epsilon_f=-1.0$ ,  $\mu=-0.4$ ,  $T=0.01$ ,

$N \times N = 32 \times 32$

# Solution to the Kondo hole problem



# Gutzwiller QP LDOS

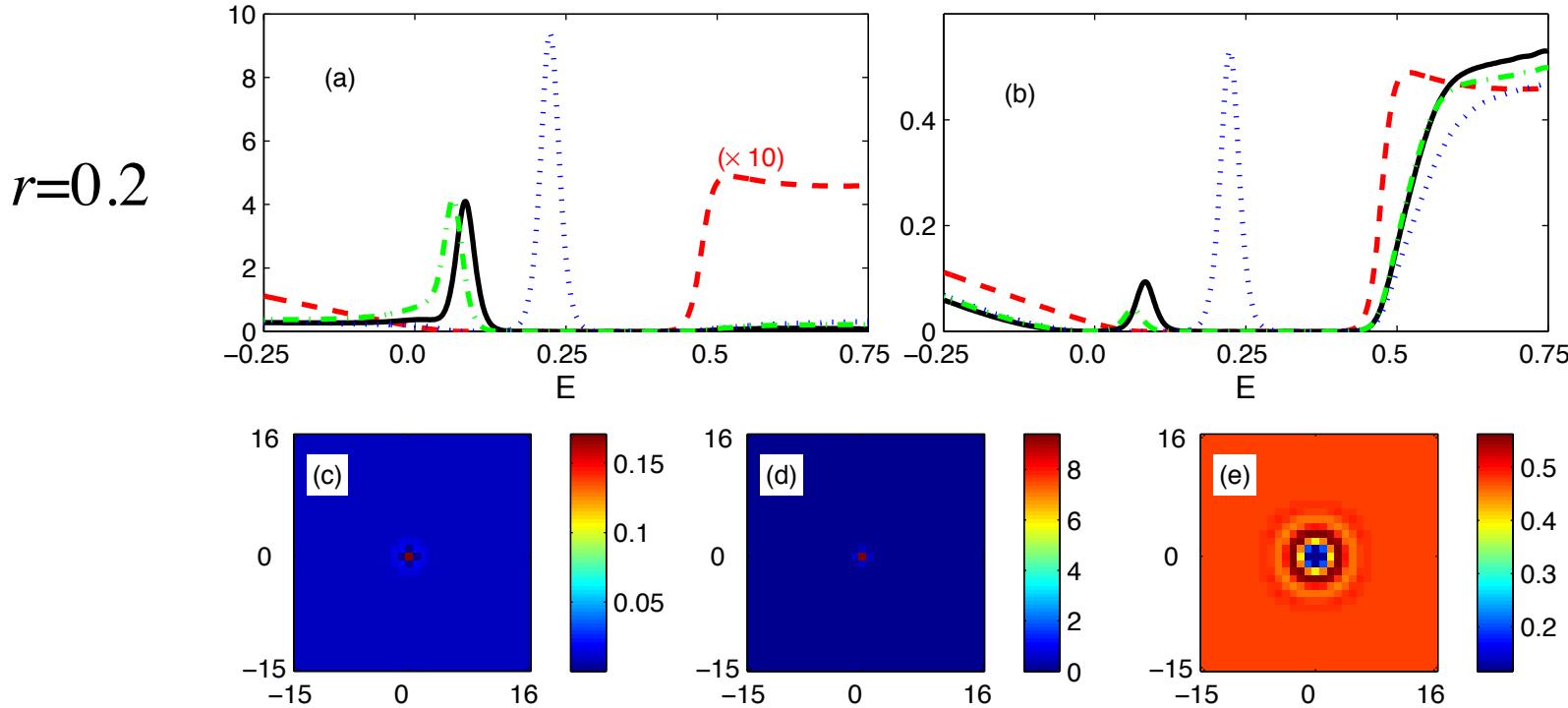


On the Kondo hole site

NN to Kondo hole site

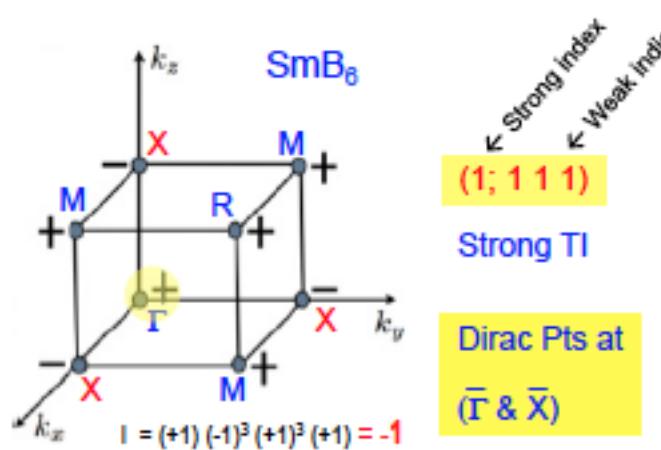


# $dI/dV$ characteristic and imaging



- Fano interference induces asymmetric  $dI/dV$ .
- Impurity bound states robust against Fano interference.

# Impurity states on the surface of TKI



- Topological index for cubic symmetry:

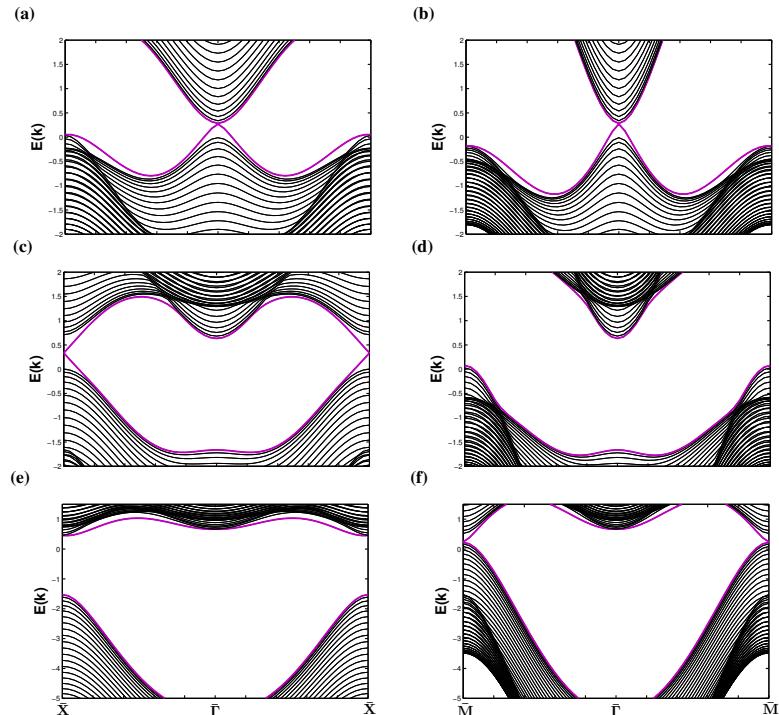
$$I = I_G \cdot I_X^3 \cdot I_M^3 \cdot I_R = \begin{cases} +1 & (\text{trivial or weak T.I.}) \\ -1 & (\text{strong T.I.}) \end{cases}$$

Dzero et al, PRL (2010)

- Single-particle surface band dispersion in TKI.
- Continuous tunability of TKI between WTKI and STKI.
- Number of Dirac cones signifies the STKI and WTKI.



Wang, Julien, JXZ, Nature Commun. (submitted)

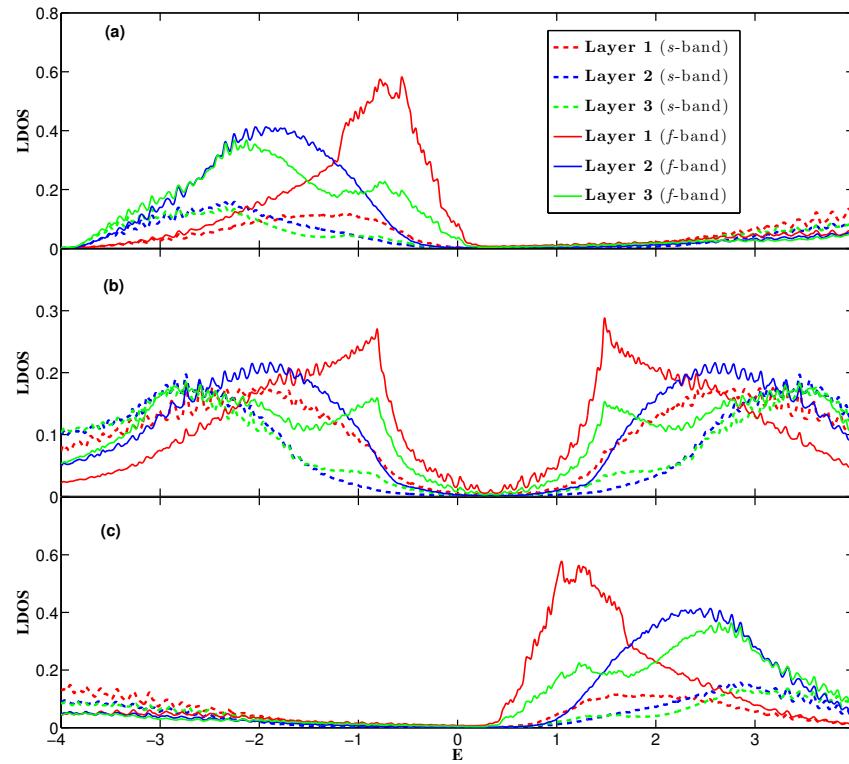


$$H_{hyb} = \sum_{ij,\sigma\alpha} \left[ c_{i\sigma}^\dagger V_{cf,ij,\sigma\alpha} f_{j\alpha} + H.c. \right]$$

$$V_{cf,ij} = d_{ij} \cdot \sigma, d_{ij} = (V_x d_{ij}^x + V_y d_{ij}^y + V_z d_{ij}^z)$$

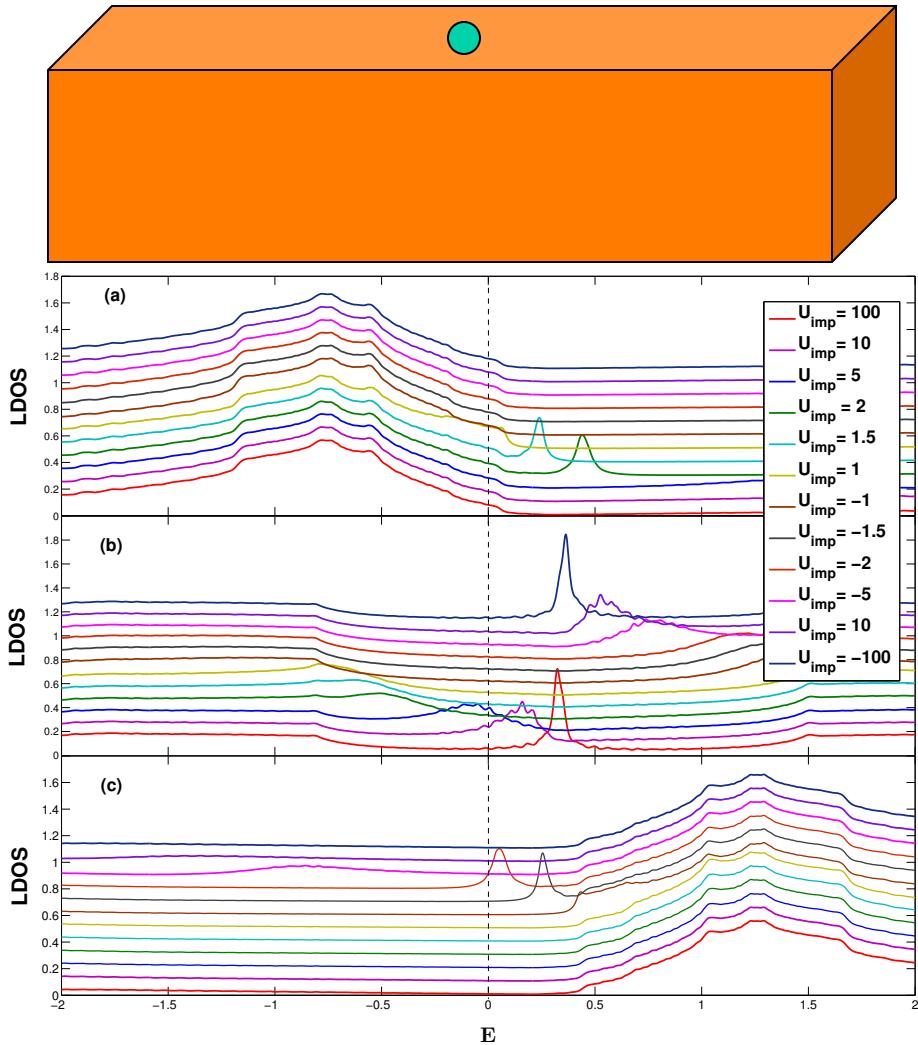


# Impurity states on the surface of TKI (II)



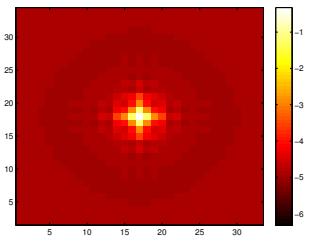
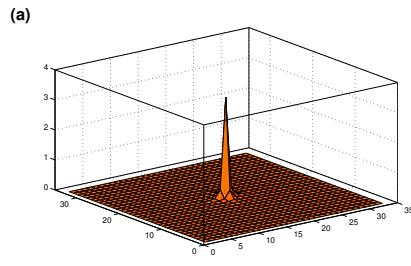
- DOS highly asymmetric w.r.t. Fermi energy for STKI state and dual nature tunable by f-electron energy level
- DOS is much less asymmetric w.r.t. Fermi energy for the WTKI state.

# Impurity states on the surface of TKI (III)

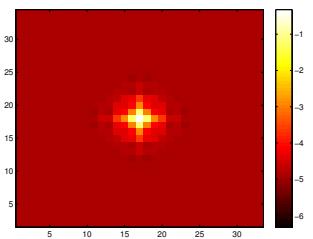
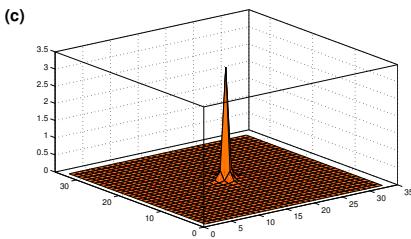
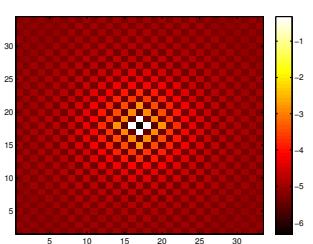
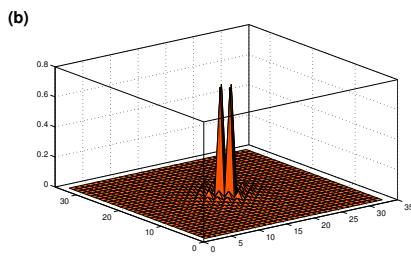


- In STKI, the impurity induced resonance peak shifts monotonically through the hybridization gap with impurity strength.
- In WTKI, the impurity induced resonance peak is moving into the hybridization gap.

# Impurity states on the surface of TKI (IV)



- LDOS imaging at resonance energy of STKI and WTKI.
- Spatial pattern also reveals the nature of TKI.



# Summary

- The Gutzwiller and related methods are powerful methods to address electronic inhomogeneity and local electronic structure in heavy fermion.
- We showcase their applications ---
  - to predict an alternative phase, Kondo stripe, as a consequence of Fermi surface mismatch;
  - to study the local electronic structure around a Kondo-hole in heavy fermion systems;
  - to address the nature of impurity induced states in relation to the topological properties of Kondo insulators.